

Supporting Information

Visible light-emitting diode light-driven one-pot four component synthesis of poly-functionalized imidazoles under catalyst and solvent-free conditions

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SI 1 General Information:

The chemicals and solvents which were utilized for the experiments reported in this manuscript were purchased from Merck, Sigma Aldrich, TCI-Chemicals, Sd-Fine and HIMEDIA (India). All the chemicals were used as received without any further purification and the solvents were distilled before used. Double distilled water is used. Organic reactions were carried out under LED light (10 W) in quartz round bottom flask. Thin layer chromatography (TLC) was carried out using pre-coated Merck made 60F254 silica gel plates with 0.25 mm breadth and ethanol was used for the recrystallization purpose.

The ¹H NMR spectra of the synthesized compounds were recorded by Bruker 500 MHz and JEOL 400MHz. The chemical shifts were recorded to the centre of solvent resonance at CDCl₃ ($\delta = 7.26$; ¹H and 77; ¹³C) for ¹H NMR studies.

SI 2: General Experimental Procedure for the synthesis of 2-aryl-1,4,5-triphenyl-1H-imidazoles: Representative experimental procedure for the synthesis of 2-phenyl-1,4,5-triphenyl-1H-imidazole (Entry 1a, Table 2):

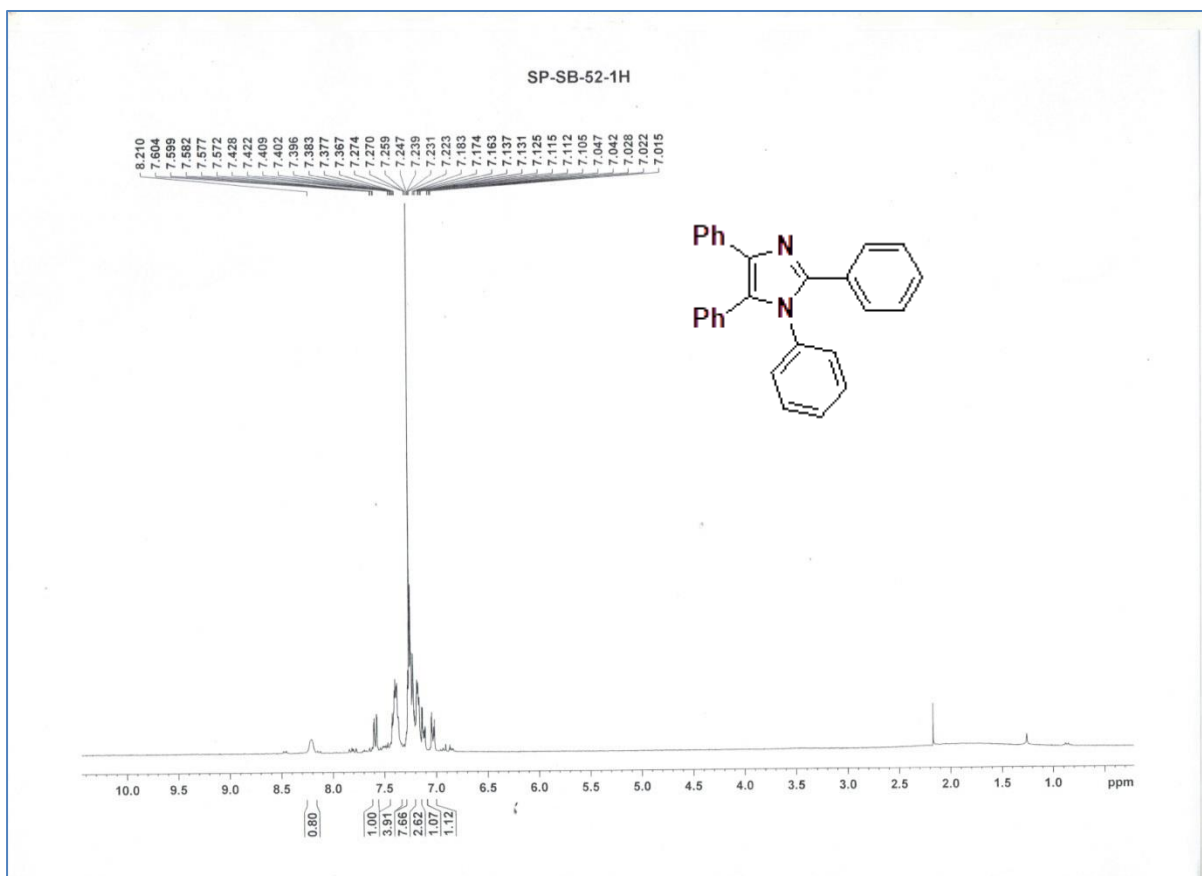
A mixture of benzil (1.0 mmol), benzaldehyde (1 mmol), ammonium acetate (1 mmol) and aniline (1 mmol) were heated at 100 °C in presence of white LED light (10 W) under neat conditions for 60 min. in a 25 ml quartz round bottom flask till completion of reaction (TLC monitored). After the completion of reaction the reaction mixture

was poured into ice-cold water which results the precipitation of imidazole derivatives. The precipitate was filtered, dried in oven and recrystallized from hot ethanol to provide pure 2-phenyl-1,4,5-triphenyl-1*H*-imidazole (**1a**) in 95% yield. The pure products were analyzed by their melting point determination (Observed: M.P: 218 -220 °C; reported 216-218 °C) and ¹H NMR spectroscopic study. The similar procedure was followed for all the reactions listed in Table 2.

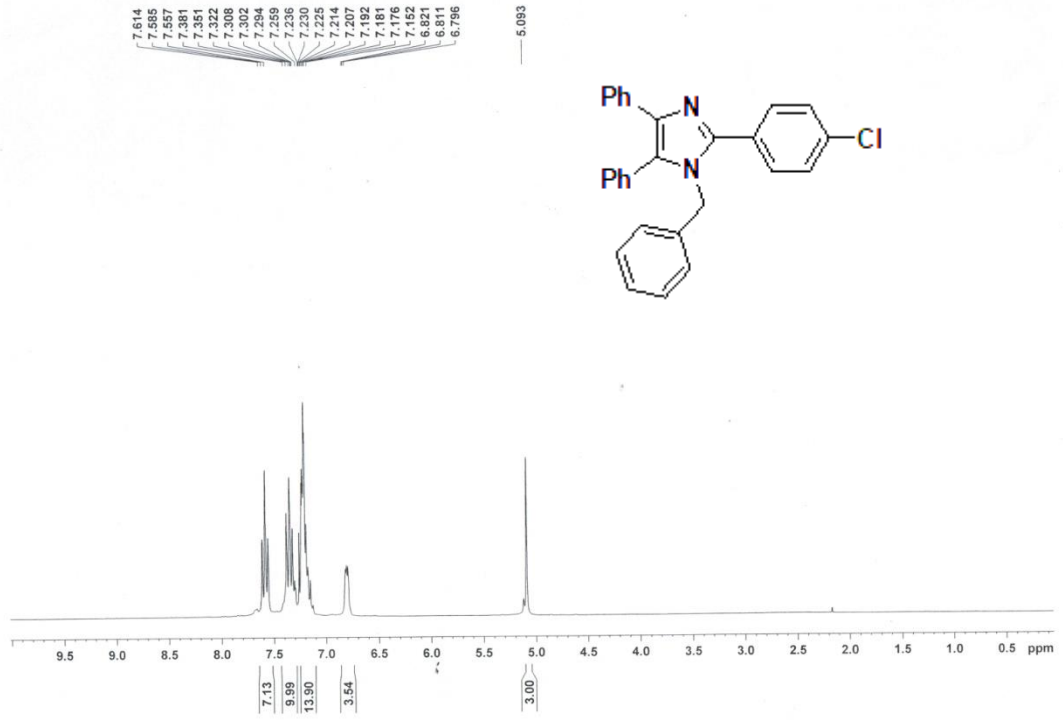
SI 3: General Experimental Procedure for the synthesis of 2-aryl-4,5-diphenyl-1*H*-imidazoles: Representative experimental procedure for the synthesis of 2-phenyl-4,5-diphenyl-1*H*-imidazole (Entry 3a, Table 3):

A mixture of benzil (1.0 mmol), benzaldehyde (1 mmol) and ammonium acetate (2 mmol) were heated at 100 °C in presence of white LED light (10 W) under neat conditions for 30 min. in a 25 ml quartz round bottom flask till completion of reaction (TLC monitored). After the completion of reaction the reaction mixture was poured into ice-cold water which results the precipitation of imidazole derivatives. The precipitate was filtered, dried in oven and recrystallized from hot ethanol to provide pure 2-phenyl-4,5-diphenyl-1*H*-imidazole (**1a**) in 98% yield. The pure products were analyzed by their melting point determination (Observed: M.P: 273 -275 °C; reported 271-273 °C) and ¹H NMR spectroscopic study. The similar procedure was followed for all the reactions listed in Table 3.

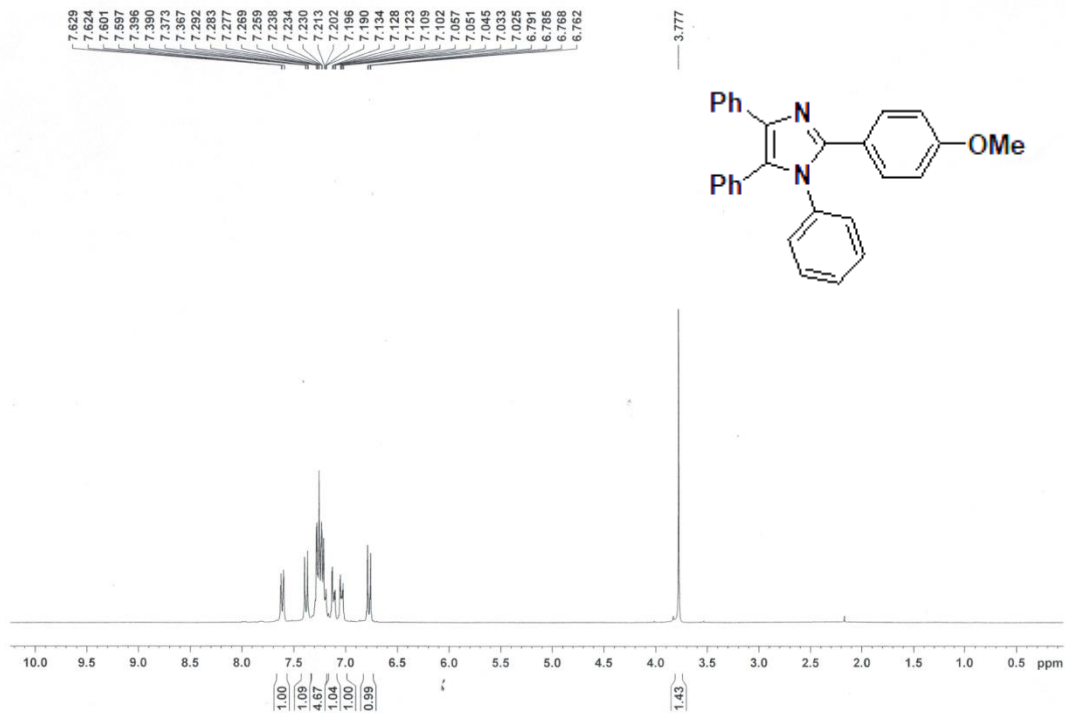
SI 4: Scan copies of ^1H NMR spectra of products listed in Table 2 and 3.



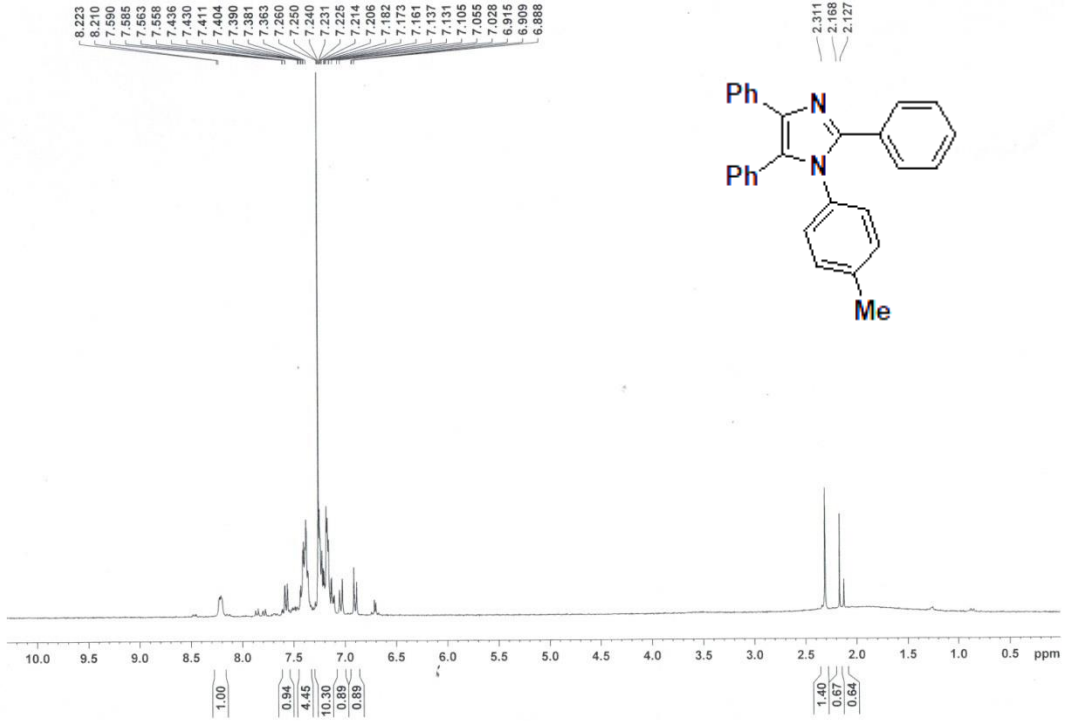
SP-SB-53-1H



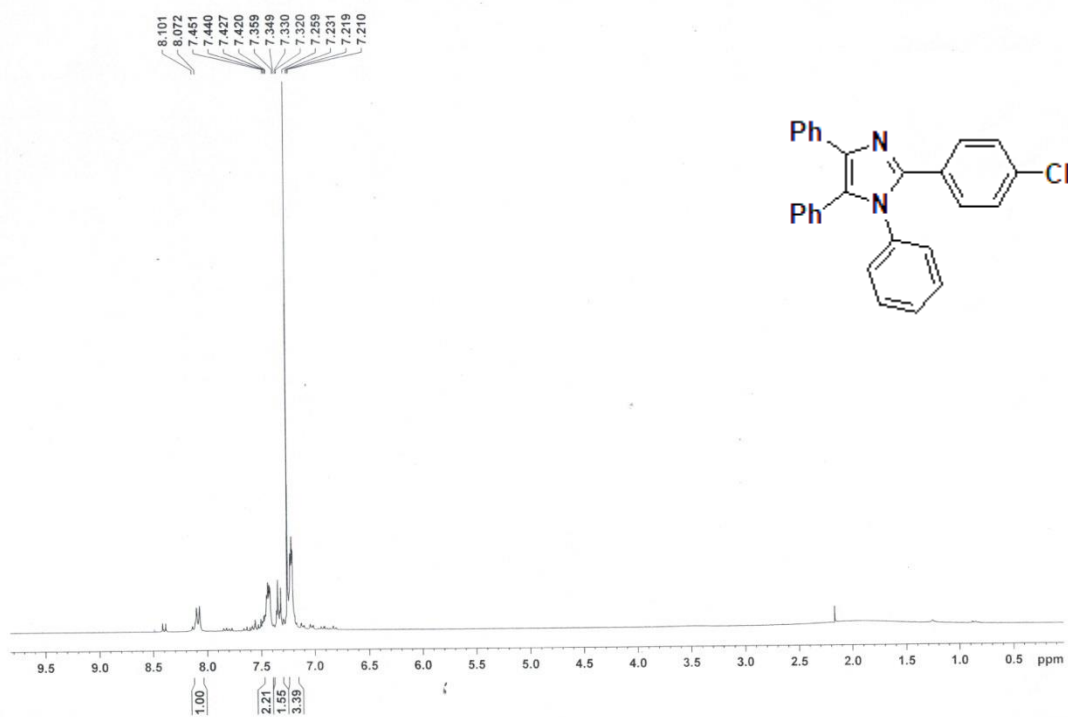
SP-SB-54-1H



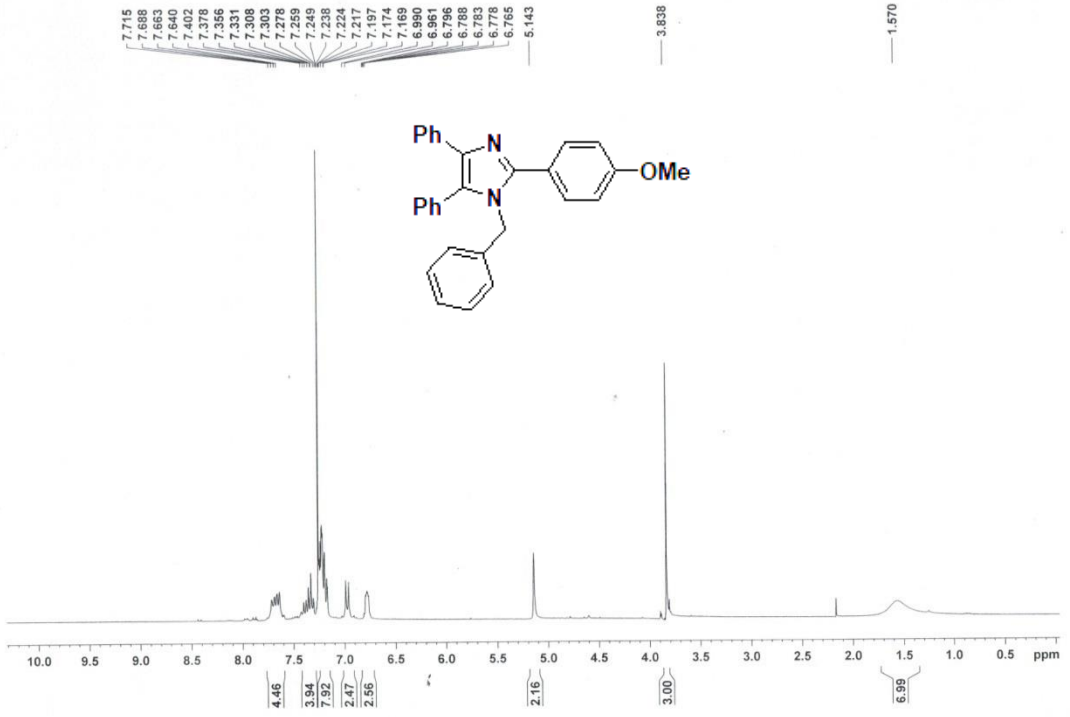
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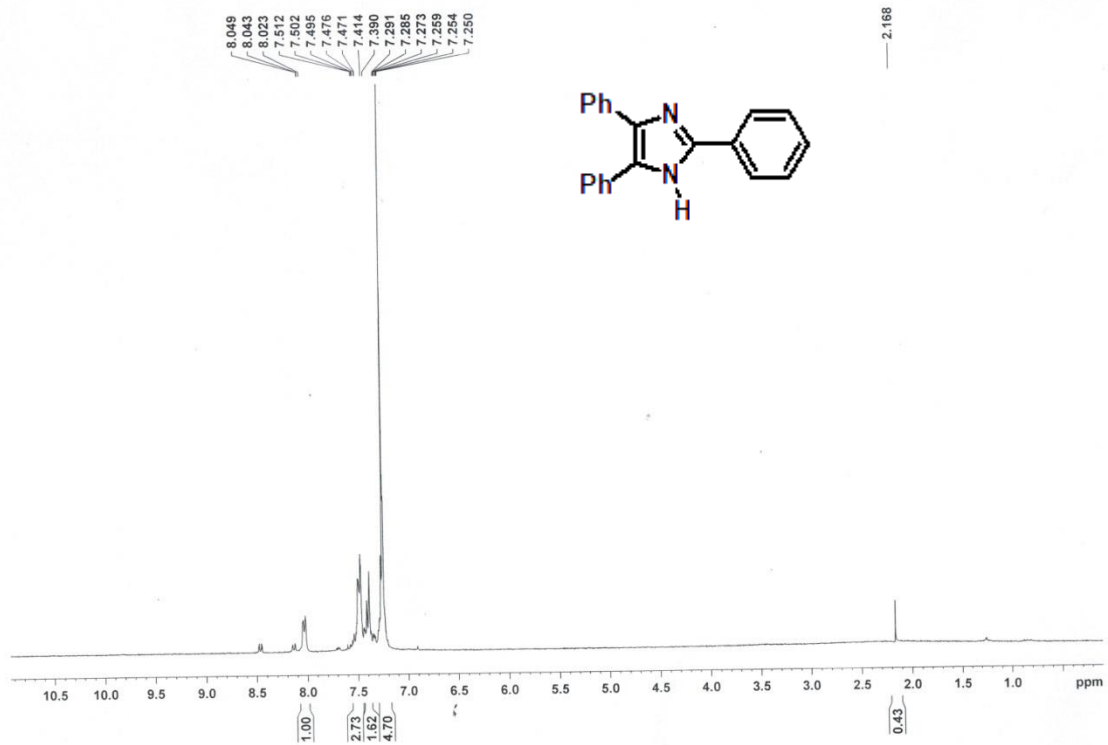
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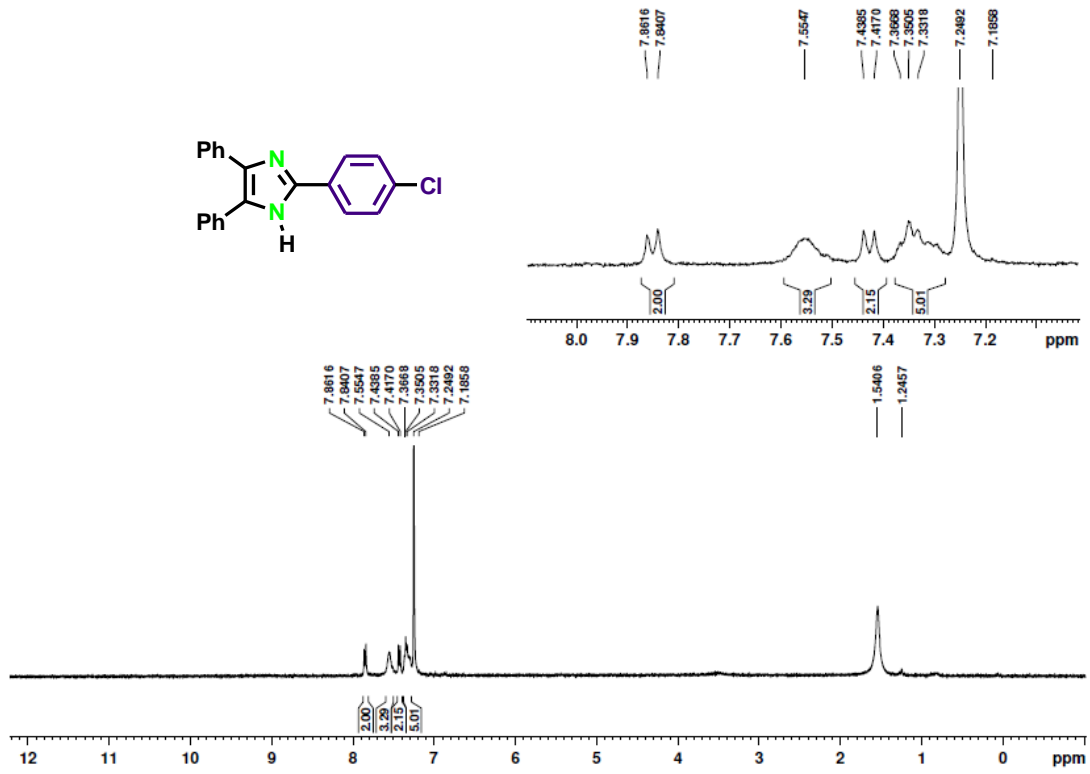
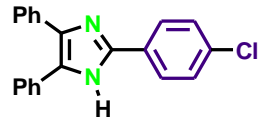
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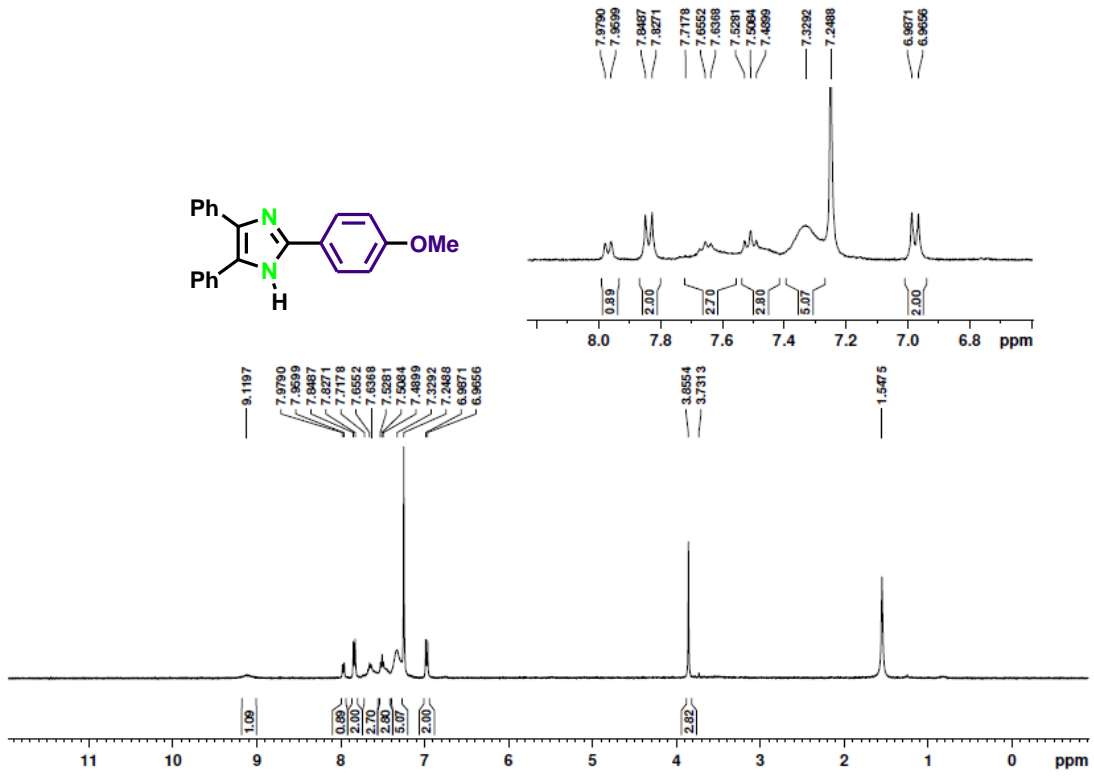
SP-SB-58-1H



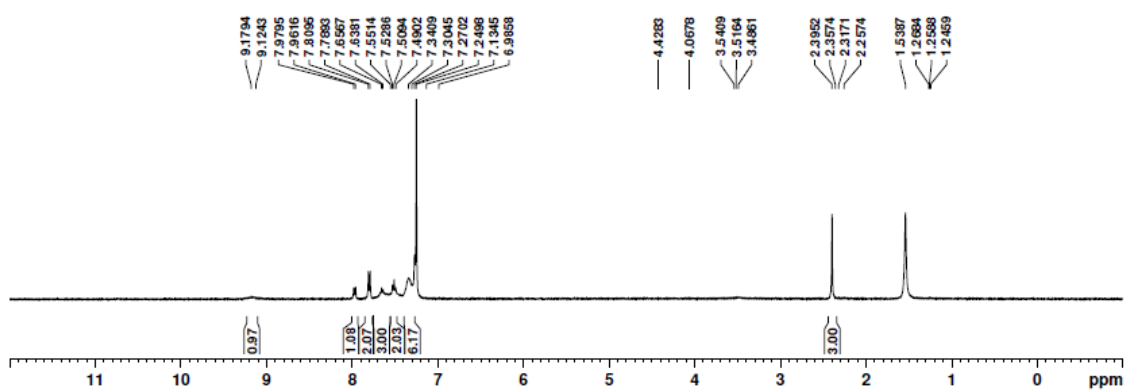
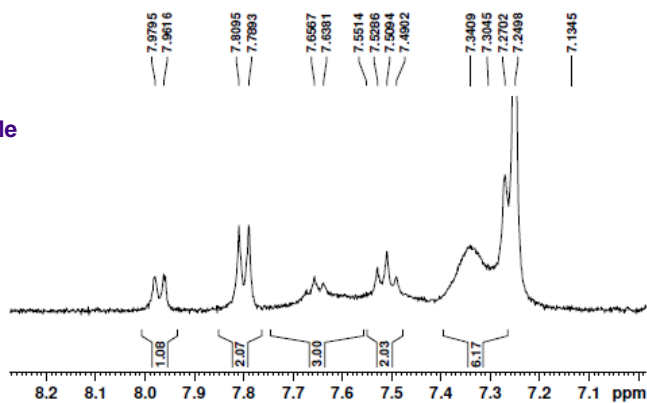
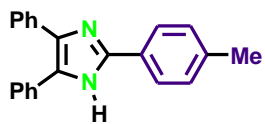
58b IN CDCl3

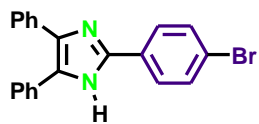


-58c IN CDCl3

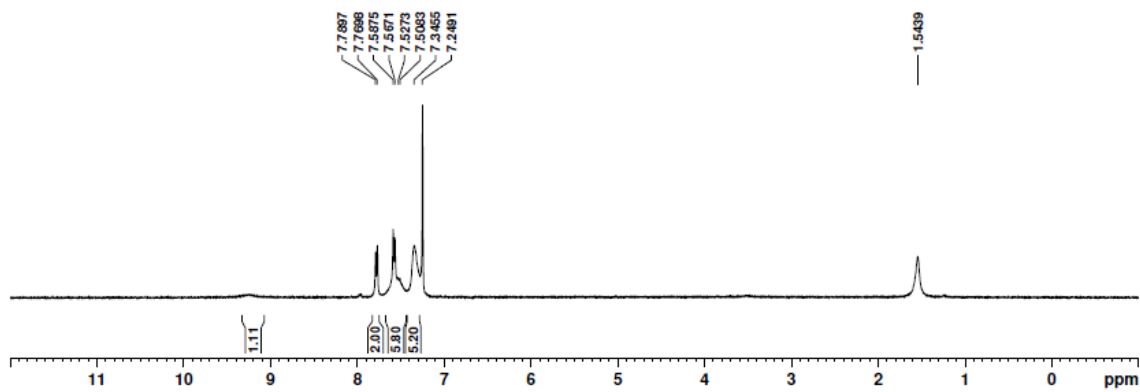
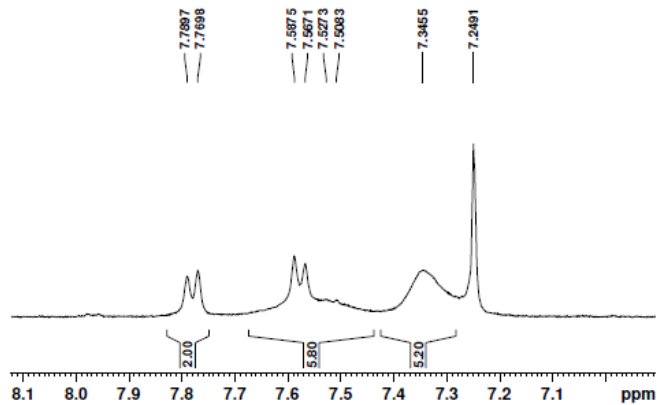


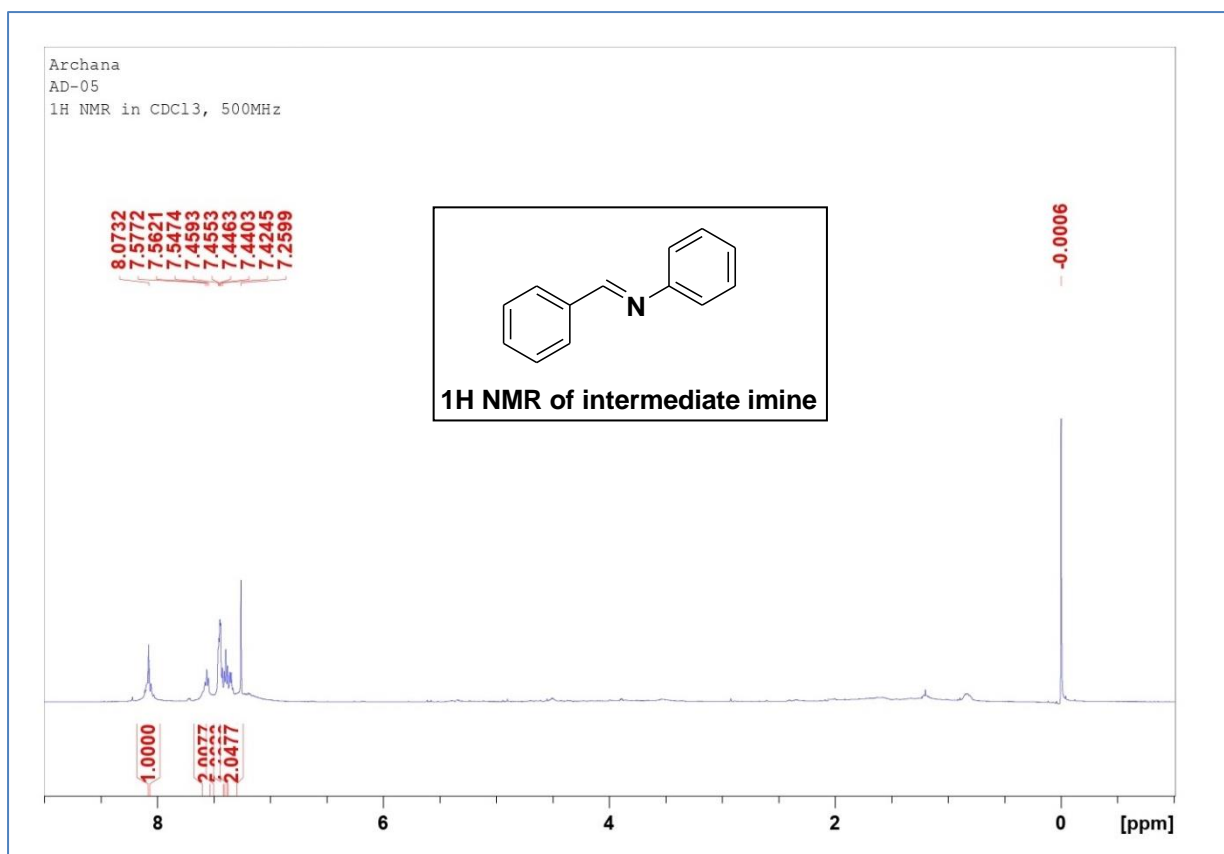
-58D IN CDCl3





-58E IN CDCl3





SI 5: Reaction set-up

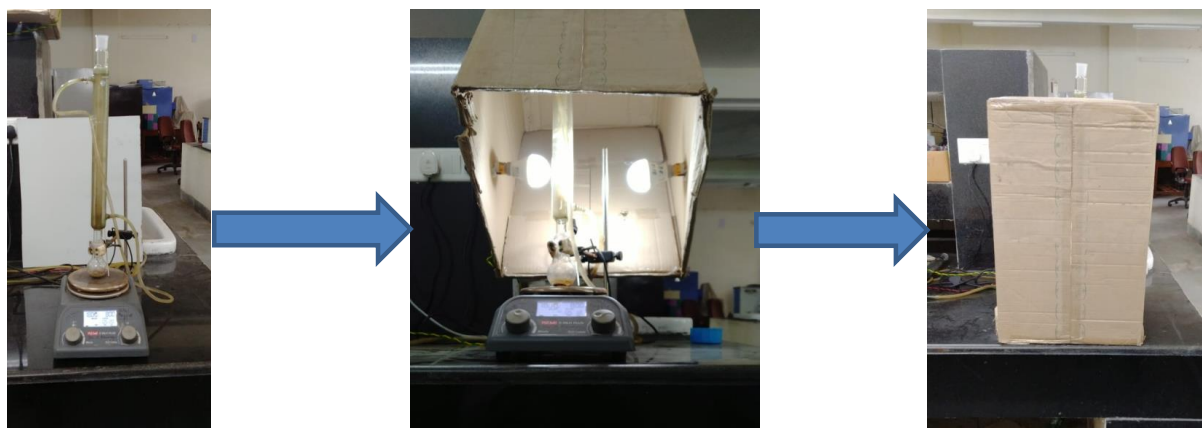


Fig. 1S Images of reaction set up